CONFORMATIONAL ANALYSIS OF γ-HEXANOLACTONE BY MICROWAVE SPECTROSCOPY

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γ-Hexanolactone (5-ethyldihydro-2-furanone) (γ-HL) is an odor molecule that is included in a natural food such as pineapple. The rotational spectra of γ-HL were observed by a Fourier transform microwave spectrometer combined with a heated nozzle of 303 K. The three conformers in expected to six were observed.For the first conformer, 65 *a*-type, 48 *b*-type, and 22 *c*-type transitions were assigned. Similarly, 41 *a*-type, 40 *b*-type, and 12 *c*-type transitions for the second one were assigned and 50 *a*-type and 34 *b*-type transitions for the third one. A comparison of the observed rotational constants with those calculated by ab initio MO method led us to conclude that the second conformer is the *eq-T* in which an ethyl group attached to C(5) is in an equatorial position (*eq*), where *T* and *G* denote the conformations about the C(6)-C(5) bond, with *T* and *G* designating *trans* and *gauche*, respectively. We identified that the first and third conformers are *eq-G'* and *eq-G*, respectively, because of absence of the *c*-type transitions and large pseudo-inertial defect for third one. The *eq-G'* of the γ-HL was calculated to be the most stable. The splittings due to internal rotation of the methyl group were observed for all the three conformers and were analyzed by the XIAM program. The rotational constants thus derived agree with the predictions made by quantum chemical calculations, MP2/6-311++G(d,p) within 0.9%.